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Weakly bound states of polar molecules in bilayers*

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Abstract We investigate a system of two polarized molecules in a layered trap. The molecules reside in adjacent layers and interact purely via the dipole-dipole interaction. We determine the properties of the ground state of the system as a function of the dipole moment and polarization angle. A bound state is always present in the system and in the weak binding limit the bound state extends to a very large distance and shows universal behavior.

Keywords dipole-dipole interaction · 2D geometry · weakly bound states · universality

1 Introduction

Cold gases of polar molecules represent an interesting opportunity to study the interplay of long- and short-range interactions in the controllable environment of the magneto-optical trap [1]. One of the possible configurations is an optical lattice with a multi-layered stack of planar traps.

We consider a system of two polar molecules in adjacent layers. The unique property of the system is that the interaction between molecules is pure dipole-dipole. This interaction has the integrated strength equal to zero – the attractive and repulsive parts of the potential are of equal integrated strength. In 2D-geometry such interaction always supports a bound state [3]. We investigate the energy and root-mean-square radius of the ground state as a function of the dipole moment and polarization angle. In particular we show that in the weak binding limit the state shows universal behavior.

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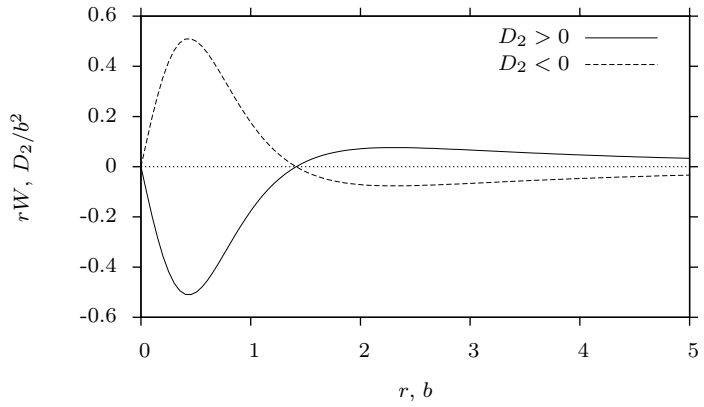

Fig. 1 The dipole-dipole potential (2) in the rotationally symmetric case, $\theta = \pi/2$, as a function of $r = \sqrt{x^2 + y^2}$. The potential is multiplied by r for better visibility.

2 The Schrödinger equation for two dipoles in bilayer geometry

The system of two polar molecules in a bilayer geometry is described by the Schrödinger equation,

$$\left[-\frac{\hbar^2}{2\mu} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) + W(x,y) \right] \psi(x,y) = E\psi(x,y) \ , \tag{1}$$

where μ is the reduced mass of the two molecules, x and y are the relative coordinates in the layer plane, and W is the dipole-dipole potential,

$$W(x,y) = D_2 \frac{x^2 + y^2 + b^2 - 3(x\cos\theta + b\sin\theta)^2}{(x^2 + y^2 + b^2)^{5/2}} \ , \tag{2}$$

where b is the distance between the layers, θ is the polarization angle measured from the layer, and D_2 is the product of the dipole moments of the molecules taken with the positive or negative sign if the dipoles are correspondingly parallel or anti-parallel.

The dipole-dipole potential has the integrated strength identically equal to zero – it has attractive and repulsive parts with equal integrated strength, see figure 1. Such a potential is expected to always have a bound state in a two-dimensional geometry [3].

3 Ground state energy

We have calculated numerically the binding energy of the ground state of the system of two polarized molecules for different dipole moments as a function of the polarization angle for parallel and anti-parallel orientation of the dipoles. The results are shown in figure 2.

For parallel dipoles the strongest binding is achieved when the dipoles are perpendicular to the layer, $\theta = \pi/2$. The binding decreases monotonically with increasing polarization angle. Approaching $\theta = 0$, the binding decreases significantly but still remains finite. For anti-parallel dipoles the situation is opposite – the binding is strongest for $\theta = 0$ and decreases towards $\theta = \pi/2$. In both cases a stronger dipole moment leads to stronger binding.

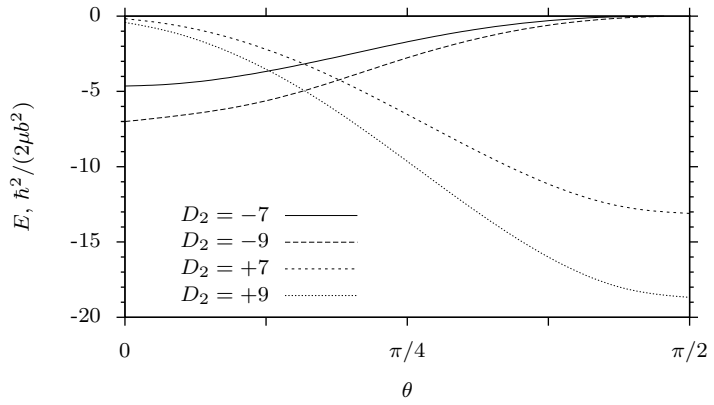

Fig. 2 Ground state energy of the system of two polar molecules described by the Schrödinger equation (1) as a function of the polarization angle θ for parallel, $D_2 > 0$, and anti-parallel, $D_2 < 0$, orientation of the dipoles. D_2 is in units of $\hbar^2 b/(2\mu)$.

4 Root-mean-square radius and universality in the weak binding limit

For short-range potentials in two dimensions the relation between the root-mean-square radius, $R_{\rm rms}$, and the binding energy, $|E|$, is universal in the limit of weak binding [4],

$$R_{\rm rms}^2 \stackrel{E\to 0}{\longrightarrow} \frac{2}{3}\frac{\hbar^2}{2\mu|E|}. \tag{3}$$

The dipole-dipole potential asymptotically decreases as r^{-3}, that is faster than the centrifugal barrier, r^{-2}. It is thus of a short-range type and must obey the universal relation. Indeed the numerical calculations show that the universal regime is approached at $|E| \sim 0.001\frac{\hbar^2}{2\mu b^2}$, see figure 3. For the parallel (anti-parallel) orientation

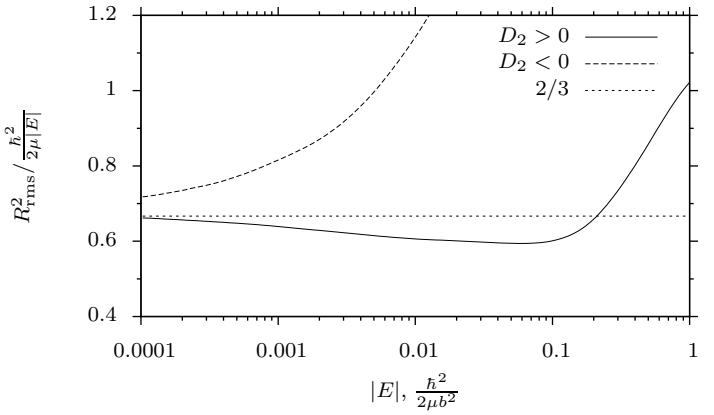

Fig. 3 Root-mean-square radius $R_{\rm rms}$ of the system of two polar molecules described by the Schrödinger equation (1) as a function of the binding energy $|E|$ for parallel, $D_2 > 0$, and anti-parallel, $D_2 < 0$, orientation of the dipoles. The binding energy was varied by changing the dipole-dipole strength D_2 while the polarization angle was fixed at $\theta = \pi/2$. The model independent (universal) asymptotic value for vanishing binding is 2/3.

of the dipoles the universal limit is reached from below (above) reflecting the geometry of the dipole-dipole potential for the two configurations – either a barrier or a core, as illustrated in figure 1.

5 Conclusion

We have investigated the ground state of a system of two polar molecules in a bilayer geometry. The ground state is always bound with the binding energy strongly dependent on the polarization angle. In the weak binding limit the system exhibits the universal relation between the root-mean-square radius and the binding energy.

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